Proceedings of the European Conference Physics of Magnetism, Poznań 2017

Strongly Anisotropic $S = 1$ (Pseudo) Spin Systems: from Mean Field to Quantum Monte-Carlo

Yu.D. Panov*, A.S. Moskvin, V.V. Konev, E.V. Vasinovich and V.A. Ulitko
Ural Federal University, Ekaterinburg 620083, Russia

The $S = 1$ pseudospin formalism was recently proposed to describe the charge degree of freedom in a model high-T$_c$ cuprate with the on-site Hilbert space reduced to the three effective valence centers, nominally $\mathrm{Cu}^{1+;2+;3+}$. With small corrections the model becomes equivalent to a strongly anisotropic $S = 1$ quantum magnet in an external magnetic field. We have applied a generalized mean-field approach and quantum Monte-Carlo technique for the model 2D $S = 1$ system to find the ground state phase with its evolution under deviation from half-filling and different correlation functions. Special attention is given to the role played by the on-site correlation ("single-ion anisotropy").

DOI: 10.12693/APhysPolA.133.426
PACS/topics: 75.10.Hk, 75.10.Jm, 74.25.Dw

1. Introduction

These days spin algebra and spin Hamiltonians are used not only in the traditional fields of spin magnetism but in so-called pseudospin lattice systems with the on-site occupation constraint. For instance, the $S = 1$ pseudospin formalism was applied to study an extended Bose-Hubbard model (EHBM) with truncation of the on-site Hilbert space to the three lowest occupation states $n = 0, 1, 2$ (semi-hard-core bosons) considered to be three pseudospin states with $M_S = -1$, $M_S = 0$, $M_S = +1$, respectively (see Ref. [1] and references therein). At variance with quantum $s = 1/2$ systems the Hamiltonian of $S = 1$ spin lattices in general is characterized by several additional terms such as a single ion anisotropy that results in their rich phase diagrams. Recently we made use of the $S = 1$ pseudospin formalism to describe the charge degree of freedom in high-T$_c$ cuprates with the on-site Hilbert space reduced to only the three effective valence centers $[\mathrm{CuO}_4]^{7-,6-,5-}$ (nominally $\mathrm{Cu}^{1+;2+;3+}$) [2–5].

2. $S = 1$ (pseudo) spin Hamiltonian

The $S = 1$ spin algebra includes the eight nontrivial independent spin operators: spin-dipole moment $\mathbf{S}$ and five spin-quadrupole operators $Q_{ij} = (\frac{1}{2}\{S_i, S_j\} - \frac{2}{3}\delta_{ij})$ whose mean values define so-called spin-nematic order. Spin operators $S_\pm$ and $T_\pm = \{S_z, S_\pm\}$ change the pseudospin projection (and occupation number!) by ± 1, while $S_\pm^2$ changes the pseudospin projection by ± 2.

Hereafter in the paper we will focus on a simplified 2D $S = 1$ (pseudo) spin Hamiltonian with the nearest neighbor coupling and the only two-particle transport term (inter-site biquadratic anisotropy) as follows:

$$\hat{H} = \sum_i (\Delta S_{iz}^2 - \mu S_{iz}) + V \sum_{\langle ij \rangle} S_{iz} S_{jz}$$
$$-t \sum_{\langle ij \rangle} (S_{i+}^2 S_{j-}^2 + S_{i-}^2 S_{j+}^2), \tag{1}$$

where $V > 0$, $t > 0$. The first single-site term in $\hat{H}$ describes the effects of a bare pseudo-spin splitting and relates with the on-site density-density interactions, or correlations: $\Delta = U/2$. The second term, or a pseudospin Zeeman coupling may be related with a pseudo-magnetic field $\| Z$ which acts as a chemical potential μ for boson systems with a boson density constraint:

$$\frac{1}{N} \sum_i \langle S_{iz} \rangle = n, \tag{2}$$

where n is the deviation from a half-filling ($n = 0$). The third (Ising) term in $\hat{H}$ describes the effects of the short- and long-range inter-site density-density interactions. The last term in $\hat{H}$ describes the two-particle inter-site hopping. In the strong on-site attraction limit of the model (large easy-axis pseudospin on-site anisotropy) we arrive at the Hamiltonian of the hard-core, or local, bosons which was earlier considered to be a starting point for explanation of the cuprate high-T$_c$ superconductivity [6]. The spin counterpart of $\hat{H}$ corresponds to an anisotropic $S = 1$ magnet with a single ion (on-site) and two-ion (bilinear and biquadratic) symmetric anisotropy in an external magnetic field. It describes an interplay of the Zeeman, single-ion and two-ion anisotropic terms giving rise to a competition of an (anti)ferromagnetic order along Z-axis with an in-plane XY spin-nematic order. A remarkable feature of the Hamiltonian (1) is that the on-site pseudospin states $M = 0$ and $|M| = 1$ do not mix under the inter-site coupling. The model allows us to directly study a continuous transformation of the semi-hard-core bosons to the effective hard-core bosons formed by boson pairs under driving the correlation parameters $\Delta = U/2$ to large negative values ("negative-U model"). The simplified model can be directly applied to a description of bosonic systems with suppressed one-particle hopping.

*corresponding author; e-mail: yuri.panov@urfu.ru

3. Mean-field approximation

To analyse the simplified model we start with a mean-field approximation (MFA) for 2D square lattice, however, at variance with a conventional classical MFA we made use of more correct approach that takes into account the quantum nature of the $S = 1$ (pseudo) spin states [7]. First we introduce a set of the on-site $S = 1$ coherent states

$$|\boldsymbol{c}\rangle = c_{-1}|-1\rangle + c_0|0\rangle + c_{+1}|+1\rangle, \tag{3}$$

where the c_M coefficients can be represented as follows

$$c_1 = \sin\frac{\theta}{2}\cos\frac{\phi}{2}\,\mathrm{e}^{-\mathrm{i}\frac{\alpha}{2}}, \quad c_0 = \cos\frac{\theta}{2}\,\mathrm{e}^{\mathrm{i}\frac{\beta}{2}},$$
$$c_{-1} = \sin\frac{\theta}{2}\sin\frac{\phi}{2}\,\mathrm{e}^{\mathrm{i}\frac{\alpha}{2}} \tag{4}$$

with $\theta, \phi, \alpha, \beta$ to be parameters defined by the minimization of the energy. The MFA energy can be written as follows

$$E = \frac{\Delta}{2}\sum_i (1-\cos\theta_i) - \frac{\mu}{2}\sum_i (1-\cos\theta_i)\cos\phi_i \tag{5}$$
$$+\frac{V}{4}\sum_{\langle ij\rangle}(1-\cos\theta_i)(1-\cos\theta_j)\cos\phi_i\cos\phi_j$$
$$-\frac{t}{8}\sum_{\langle ij\rangle}(1-\cos\theta_i)(1-\cos\theta_j)\sin\phi_i\sin\phi_j\cos(\alpha_i-\alpha_j).$$

It is worth noting that due to the absence of the one-particle inter-site hopping terms in Hamiltonian (1) the energy does not depend on phase parameter β, so the β remains undetermined. Below we denote $\delta = \Delta/t$ and $v = V/t$. In a two-sublattice A-B model we arrive at a high-temperature non-ordered (NO) phase and the five MFA uniform phases, two phases with nonzero local superfluid order parameter, or pseudospin nematic order $\langle S^2_{A,B\pm}\rangle \neq 0$ and three charge ordered phases with $\langle S^2_{A,B\pm}\rangle = 0$ but different types of the sublattice occupation (pseudospin S_z components):

Superfluid (SF) phase: $\langle S_{A,Bz}\rangle = n$, $\langle S^2_{A,Bz}\rangle = 1$, $\langle S^2_{A,B\pm}\rangle = \frac{\zeta}{2}\sqrt{1-n^2}e^{\pm i\alpha}$, uncertain factor $\zeta = \pm 1$.

Supersolid (SS) phase: $\langle S^2_{A,Bz}\rangle = 1$, $\langle S_{A,Bz}\rangle = n \mp \sqrt{1+n^2-\frac{4|n|\nu}{\sqrt{4\nu^2-1}}}$, $\langle S^2_{A,B\pm}\rangle = \frac{\zeta}{2}e^{\pm i\alpha}\left(\sqrt{|n|\sqrt{\frac{2\nu+1}{2\nu-1}}-n^2} \pm \operatorname{sgn} n\sqrt{|n|\sqrt{\frac{2\nu-1}{2\nu+1}}-n^2}\right)$.

Charge ordered COI phase: $\langle S_{Az}\rangle = 0$, $\langle S^2_{Az}\rangle = 0$, $\langle S_{Bz}\rangle = 2n$, $\langle S^2_{Bz}\rangle = 2|n|$, $(|n| \leqslant 0.5)$.

Charge ordered COII phase: $\langle S_{Az}\rangle = 2n - \operatorname{sgn} n$, $\langle S^2_{Az}\rangle = 1-2|n|$, $\langle S_{Bz}\rangle = \operatorname{sgn} n$, $\langle S^2_{Bz}\rangle = 1$, $(|n| \leqslant 0.5)$.

Charge ordered COIII phase: $\langle S_{Az}\rangle = \operatorname{sgn} n$, $\langle S^2_{Az}\rangle = 1$, $\langle S_{Bz}\rangle = 2n - \operatorname{sgn} n$, $\langle S^2_{Bz}\rangle = 2|n| - 1$, $(|n| \geqslant 0.5)$.

Interestingly, all the local order parameters do not depend on the correlation parameter Δ, while this parameter governs the energy of different phases. Taking into account the on-site correlations we arrive at very rich and intricate phase diagrams for the model system as compared with relatively simple phase diagrams for hard-

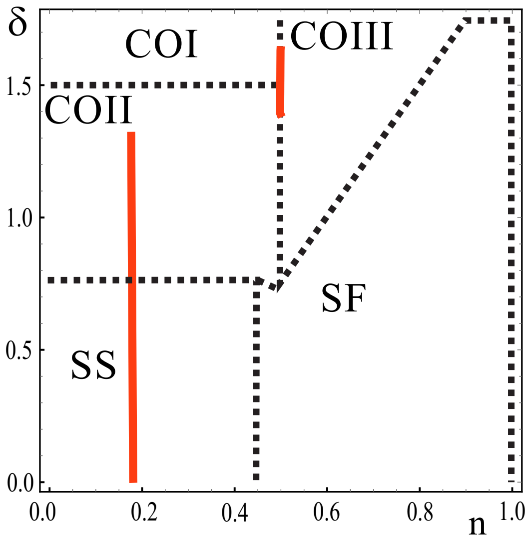

Fig. 1. The δ-n ground state phase diagrams for the model system given $V/t = 0.75$ (dotted lines are the MFA results, solid lines are the QMC results).

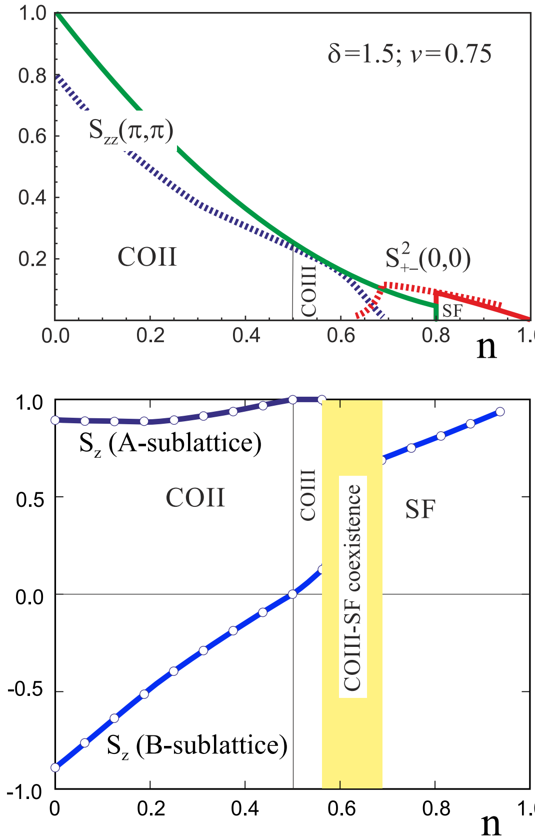

Fig. 2. Top panel: Correlation functions for the model S=1 pseudospin system given $\Delta/t = 1.5$, $V/t = 0.75$, solid lines are the MFA results, dotted lines are the QMC results. Bottom panel: QMC data for the sublattice S_z-components as functions of the deviation from the half-filling. Filling points to a COIII-SF coexistence phase typical for the first kind phase transition.

core bosons [6, 8]. In Fig. 1 (dotted curves) we present an example of the MFA $\delta - n$ phase diagrams calculated given $v = 0.75$. At half-filling $n = 0$ the positive values of the correlation parameter δ stabilize a limiting COI phase with $\langle S_{A,Bz}\rangle = \langle S^2_{A,Bz}\rangle = 0$, or a "parent Cu^{2+} phase" for a model cuprate, while positive values of v stabilize a limiting COII phase with $\langle S_{A,Bz}\rangle = \pm 1$; $\langle S^2_{A,Bz}\rangle = 1$, or a checkerboard "antiferromagnetic" order of pseudospins along z-axis, or a disproportionated Cu^{1+}-Cu^{3+} phase for a model cuprate. As a result of the competition between the on-site and inter-site correlations we arrive at a "starting" COI phase for $\delta > 2v$ or COII phase for $\delta \leqslant 2v$. At n=0.5 we see a transformation of the COI and COII phases into the COIII phase. The line of the first order phase transition COIII-SF in Fig. 1 corresponds to the equality of the respective energies. It is worth to note that the critical concentration n for the SS-SF, COI, COII-COIII transitions does not depend on the correlation parameter δ. In Fig. 2 (top panel, solid lines) we present the n-dependence of the correlation functions $S_{zz}(\pi,\pi)$=$\langle S_z, S_z\rangle$ (static structure factor) and $S^2_{+-}(0,0)$=$\langle S^2_+, S^2_-\rangle$ at δ=1.5, v=0.75, determining the long-range CO and SF orders, respectively, given $\Delta/t = 1.5$, that is in an immediate closeness to COII-COI phase transition for small n.

4. Quantum Monte-Carlo calculations

We have performed Quantum Monte-Carlo (QMC) [9] calculations for our model Hamiltonian (1). In Fig. 1 (solid lines) we compare the ground state $\delta - n$ phase diagram of our model 2D system calculated on square lattice 8×8 given $v = 0.75$ with that of calculated within MFA approach. As for simple hard-core counterpart [6,8], despite some qualitative agreement, we see rather large quantitative difference between two curves in Fig. 1. In particular, it concerns a clearly larger volume of the quantum SF phase that might be related with a sizeable suppression of quantum fluctuations within MFA approach. In Fig. 2 (top panel, two dotted lines) we present the QMC calculated static structure factor $S_{zz}(\pi,\pi)$ and the superfluid (pseudospin nematic) correlation function $S^2_{+-}(0,0)$. It is worth to note a semiquantitative agreement with the MFA data. Smaller value of the quantum structure factor $S_{zz}(\pi,\pi)$ at n=0 is believed to be a result of the pseudospin reduction due to quantum fluctuations. Bottom panel in Fig. 2 shows the n-dependence of the mean sublattice S_z values, S_{Az} and S_{Bz}, that clearly demonstrates the pseudospin quantum reduction effect within COII phase and specific features of the sublattice occupation, or "pseudo-magnetization" under COII-COIII-SF transformation.

5. Conclusions

A simplified 2D $S = 1$ pseudospin Hamiltonian with a two-particle transport term (pseudospin nematic coupling) was analyzed within a generalized MFA and QMC technique.

Acknowledgments

The research was supported by the Government of the Russian Federation, Program 02.A03.21.0006 and by the Ministry of Education and Science of the Russian Federation, projects Nos. 2277 and 5719.

References

[1] A.S. Moskvin, *JETP* **121**, 477 (2015).

[2] A.S. Moskvin, *Phys. Rev. B* **84**, 075116 (2011).

[3] A.S. Moskvin, *J. Phys.:Condens. Matter* **25**, 085601 (2013).

[4] A.S. Moskvin, *J. Phys.: Conf. Ser.* **592**, 012076 (2015).

[5] A.S. Moskvin, Yu.D. Panov, F.N. Rybakov, A.B. Borisov, *J. Supercond. Nov. Magn.* **30**, 43 (2017).

[6] R. Micnas, J. Ranninger, S. Robaszkiewicz, *Rev. Mod. Phys.* **62**, 113 (1990).

[7] N.A. Mikushina, A.S. Moskvin, *Phys. Lett. A* **302**, 8 (2002).

[8] G. Schmid, S. Todo, M. Troyer, A. Dorneich, *Phys. Rev. Lett.* **88**, 167208 (2002).

[9] V.G. Rousseau, *Phys. Rev. E* **78**, 056707 (2008).